

s7.m24.o3 **Crystal Structures of 1,5,9,18,22,26-Hexaaza[11.11]-*p*-cyclophane Adducts; Two-dimensional Supramolecular Networks.** Teresa Borowiak, Maciej Kubicki, Grzegorz Dutkiewicz, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland; e-mail: borowiak@amu.edu.pl

Keywords: Macrocyclic Amines; Weak and Strong Acid Adducts of; Two-Dimensional Supramolecular Frameworks

The adduct formed between 1,5,9,18,22,26-hexaaza[11.11]-*p*-cyclophane, $C_{28}H_{46}N_6$, and *o*-nitrophenol is a salt $(C_{28}H_{50}N_6)^{4+} \cdot 4 (C_6H_4NO_2O)^-$ (1), and the adduct formed by the same macrocyclic amine with HCl is an aquated salt $(C_{28}H_{52}N_6)^{6+} \cdot 6Cl^- \cdot 4H_2O$ (2). The conformations of the macrocycles in (1) and (2) are different. In (1) the tetra-protonated cations lie across centres of inversion whereas in (2) the hexa-protonated cations occupy planes of symmetry. In (1) the ionic synthon is formed by two macrocyclic cations and four phenolate anions linked by strong hydrogen bonds $N^+ \cdots H \cdots O$ that close two eight-membered rings (Fig. 1). Each of them is formed by four hydrogen bonds. This association expands into heterogenic chains formed by macrocyclic cations and phenolate anions. The last ones form also homogenic chains connected by weak hydrogen bonds $C-H \cdots O$ which expand into sheets through the eight-membered hydrogen-bonded rings. The supramolecular structure thus formed is two-dimensional, each macrocyclic cation participates in two sheets through the eight-membered rings. The supramolecular units interact only by weak, non-specific van der Waals forces.

In (2) the ionic synthon is built from one macrocyclic hexa-protonated amine and six chloride anions (Fig. 2). Each anion is linked to two neighbouring cations by strong hydrogen bonds $N^+ \cdots H \cdots Cl^-$ thus generating continuous sheets with two different kinds of channels. In one of them the Cl^- anions are located, in the other – the disordered water molecules. A three-dimensional framework is created by stacks of sheets with only weak van der Waals interactions between them.

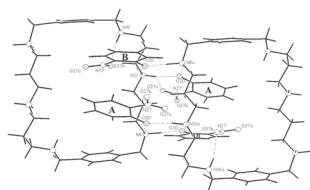


Fig. 1. The ionic synthon of (1)

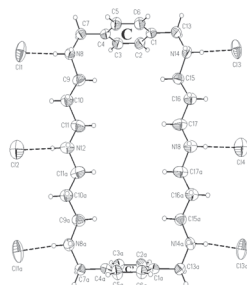


Fig. 2. The ionic synthon of (2)

s7.m24.o4 **Are Predicted Structures High Pressure Polymorphs?** Iain D.H. Oswald, Simon Parsons, David R. Allan and W.D.Samuel Motherwell, University of Edinburgh, Science and Engineering, Chemistry, West Mains Road, Edinburgh, UK. E-mail: iain.oswald@ed.ac.uk

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In 1999 and 2001 the Cambridge Crystallographic Data Centre held blind tests of crystal structure prediction. The aim of these projects was ‘...to test how well currently available methods of crystal structure prediction perform when given only the atomic connectivity for an organic compound’.

The results from the tests were fairly ‘unsuccessful’ at predicting the ambient crystal structure, except in a handful of cases. The CCDC blind tests compared the predicted structures with the experimental results obtained from certain crystallisation conditions. It is a well-known fact that some molecules can adopt many different polymorphs depending on the conditions of growth. Another technique that we have been developing in Edinburgh is the use of high-pressure as a way of accessing new polymorphs. Can we access new high-pressure polymorphs that correspond to predicted structures? Are predicted structures high-pressure polymorphs?